

# PROJECT facts

U.S. DEPARTMENT OF ENERGY  
OFFICE OF FOSSIL ENERGY  
NATIONAL ENERGY TECHNOLOGY LABORATORY

Sequestration

12/2004



## CONTACTS

### Scott M. Klara

Sequestration Technology Manager  
National Energy Technology Laboratory  
626 Cochran's Mill Road  
P.O. Box 10940  
Pittsburgh, PA 15236  
412-386-4864  
[scott.klara@netl.doe.gov](mailto:scott.klara@netl.doe.gov)

### David A. Lang

Project Manager  
National Energy Technology Laboratory  
626 Cochran's Mill Road  
P.O. Box 10940  
Pittsburgh, PA 15236  
412-386-4881  
[david.lang@netl.doe.gov](mailto:david.lang@netl.doe.gov)

### Beth McCulloch

External Technology Specialist  
UOP LLC  
50 East Algonquin Road  
Des Plaines, IL 60016  
847-391-2653  
[Beth.McCulloch@uop.com](mailto:Beth.McCulloch@uop.com)

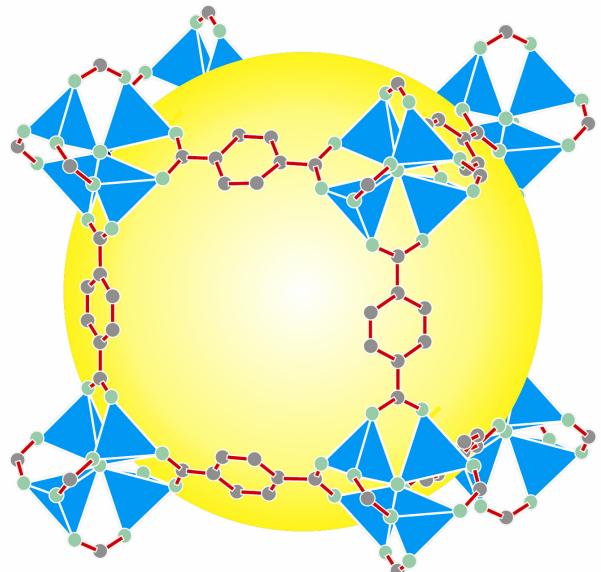
## CARBON DIOXIDE SEPARATION WITH NOVEL MICROPOROUS METAL ORGANIC FRAMEWORKS

### Background

UOP LLC, the University of Michigan, and Northwestern University are collaborating on a three-year program to develop novel microporous metal organic frameworks (MOFs) suitable for CO<sub>2</sub> capture and separation. MOFs are hybrid organic/inorganic structures in which the organic moiety is readily derivatized. This innovative program is using sophisticated molecular modeling to evaluate the structurally diverse, highly porous, thermally stable MOFs, which have shown exceptional storage capacity for methane. Selected MOFs will be optimized for CO<sub>2</sub> selectivity, adsorption capacity, and rates of adsorption and desorption.

This partnership of industry and university researchers brings a novel approach and unique depth of experience to the problem of CO<sub>2</sub> separation and capture. The University of Michigan has extensive experience in the discovery and tailoring of novel MOFs for adsorption of gases, such as methane and hydrogen. In this proposal, the use of MOFs will be extended to CO<sub>2</sub> separation. UOP is a global leader in process chemistry and has developed a broad portfolio of technologies for separating CO<sub>2</sub> from gas streams. Northwestern University will be consulting on molecular modeling.

*Molecular structure of the microporous metal organic frameworks (MOFs)*



## CUSTOMER SERVICE

1-800-553-7681

## WEBSITE

[www.netl.doe.gov](http://www.netl.doe.gov)

## PARTNERS

UOP LLC

University of Michigan

Northwestern University

## COST

### Total Project Value

\$900,000

### DOE/Non-DOE Share

\$900,000/\$0

MOFs are a structurally diverse family of materials with over 500 having been prepared. The proposed technical approach is to use molecular modeling to identify MOFs with the best sorption properties for CO<sub>2</sub> and to predict the structures of new MOFs. Synthesis of the organic linker is an important part of the preparation of novel MOFs. In addition, detailed characterization of the novel materials will be performed to determine the active sorption sites. UOP will perform process modeling and economic analysis of processes designed for the separation and capture of CO<sub>2</sub> from gas mixtures produced by electric utilities.

The core technologies are supported by academic and industrial experience in materials development, materials characterization, and process modeling. Professor Yaghi, from the University of Michigan, brings an in-depth understanding on developing new material topologies with high structural stability, high porosity, and variable pore size and porosity. UOP has a unique capability to understand commercial requirements and to deliver technology and will use these skills to integrate MOF technology into a process for the capture of CO<sub>2</sub> from flue gas and gasifier streams.

## Primary Project Goal

The primary goal of this project is to develop a low-cost, novel sorbent to remove CO<sub>2</sub> from flue gas and gasifier streams in coal-fueled power plants. The sorbent will have high selectivity, high adsorption capacity, and good adsorption/desorption rates. In addition, the MOFs will be tailored to minimize the CO<sub>2</sub> binding energy in an effort to reduce the energy required for regeneration.

## Objectives

The objectives of the program are:

- To develop a theoretical model to predict the structure of MOFs with good CO<sub>2</sub> sorption properties. This model will allow for the efficient screening of existing MOFs and for the design of new MOFs and the prediction of their sorption properties.
- To develop an understanding of the sorption sites in MOFs.
- To develop MOFs tailored for CO<sub>2</sub> separation from flue gas.
- To develop MOFs tailored for CO<sub>2</sub> separation from gasifier streams.
- To assess the commercial potential of MOFs for separation and capture of CO<sub>2</sub>.
- To integrate an MOF-based process into a coal-fueled power plant to recover CO<sub>2</sub> from actual plant-generated gas mixtures.

## Benefits

Although oil production in the U.S. has been gradually declining, we have huge reserves of coal. Unfortunately, when coal is burned, it releases more CO<sub>2</sub> per unit of heat than any other fossil fuel, and anthropogenic CO<sub>2</sub> is believed to be contributing to global warming and climate change. Successful completion of this program could lead to a low-cost, novel sorbent to remove CO<sub>2</sub> from flue gas and gasifier streams in electric power plants. The captured CO<sub>2</sub> could then be sequestered to prevent its emission to the atmosphere. This would enable the use of our coal reserves as an energy source without contributing to global warming, while simultaneously creating jobs and reducing our dependence on imported oil.